

Message

From: onbehalfof+ehpmanuscripts+niehs.nih.gov@manuscriptcentral.com
[onbehalfof+ehpmanuscripts+niehs.nih.gov@manuscriptcentral.com]
on behalf of ehpmanuscripts@niehs.nih.gov [ehpmanuscripts@niehs.nih.gov]
Sent: 11/2/2015 2:46:01 PM
To: Cogliano, Vincent [/o=ExchangeLabs/ou=Exchange Administrative Group
(FYDIBOHF23SPDLT)/cn=Recipients/cn=51f2736376ac4d32bad2fe7cfef2886b-Cogliano, Vincent]
Subject: Invitation to Review 15-10909-ART for EHP

02-Nov-2015

Dear Dr. Cogliano:

Manuscript ID 15-10909-ART titled "Prioritizing Chemicals for Risk Assessment Using Chemoinformatics: Examples from the IARC Monographs on Pesticides" by Guha, Neela; Guyton, Kathryn; Loomis, Dana; Barupal, Dinesh has been submitted to Environmental Health Perspectives.

I invite you to review this manuscript. The abstract appears at the end of this letter. Please let me know as soon as possible if you will be able to accept my invitation to review. We prefer to receive review comments within two weeks of accepting the invitation, but if you need extra time please let us know and we can adjust the due date.

If you are unable to review at this time, I would appreciate you recommending another expert reviewer. Recommendations for alternate reviewers should be e-mailed to EHPManuscripts@niehs.nih.gov. Please be sure to reference the correct manuscript number in the subject field of your e-mail.

By clicking the appropriate link at the bottom of the page, your reply will be automatically registered with our online manuscript submission and review system.

If you accept my invitation to review this manuscript, you will be notified via e-mail about how to access Manuscript Central, our online manuscript submission and review system. You will then have access to the manuscript and reviewer instructions in your Reviewer Center.

I realize that our expert reviewers greatly contribute to the high standards of the Journal, and I thank you for your present and/or future participation.

Sincerely,

Dr. Manolis Kogevinas
Environmental Health Perspectives
ehpmanuscripts@niehs.nih.gov

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MANUSCRIPT DETAILS

TITLE: Prioritizing Chemicals for Risk Assessment Using Chemoinformatics: Examples from the IARC Monographs on Pesticides

ABSTRACT: Identifying cancer hazards is the first step towards cancer prevention. The IARC Monographs Programme, which has evaluated nearly 1000 agents for carcinogenic potential since 1971, typically selects agents for hazard identification on the basis of public nominations, expert advice, published data on carcinogenicity, and public health importance. Here we present a novel and complementary strategy for identifying agents for hazard evaluation using chemoinformatics, database integration and automated text mining. To inform selection among a broad range of pesticides nominated for evaluation, we identified and screened nearly 6000 relevant chemical structures, thereafter systematically compiled information on 980 pesticides, creating chemical similarity network maps that allowed cluster visualization by chemical similarity, class, and the number of publications concerning epidemiology, cancer bioassays, and carcinogenic mechanisms. For the IARC Monograph meetings that took place in March and June 2015, this approach supported high priority evaluation of glyphosate, malathion, parathion, tetrachlorvinphos, diazinon, DDT, lindane, and 2,4-D. This systematic approach, accounting for chemical similarity and overlaying multiple data sources, can be used by risk assessors as well as researchers to systematize, inform and increase efficiency in selecting and prioritizing agents for hazard identification, risk assessment, regulation or further investigation. This approach could be extended to an array of outcomes and agents, including occupational carcinogens, drugs, and foods.